Mixed-Domain and Reduced-Order Modeling of Electroosmotic Transport in Bio-MEMS

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Abstract

A popular mechanism for transport of biological and non-biological fluidic samples in micro-scale geometries is the use of electrical fields. The use of electrical potentials to transport fluids is referred to as electroosmosis. In this paper, we present theories and results for electroosmotic transport in Bio-MEMS applications. In particular, we will describe approaches for efficient mixed-domain simulation of electroosmotic transport, and the extraction of reduced-order or low-order models for electroosmotic transport.

1   Introduction

Within the rapidly growing realm of microelectromechanical systems(MEMS), biological systems such as micro-total analysis systems(μTAS) have received a lot of attention in recent years [1]. Electrokinetic transport is typically utilized both to drive fluids through these systems and to separate different components of a sample. Cost-effective design and fabrication of these devices requires computationally efficient simulation tools. Currently, these tools use mesh-based methods such as finite element and finite difference methods to solve the governing partial differential equations.

Meshless methods require that the domain be defined only by a point distribution with no connectivity information needed. Such methods are especially appealing for the emerging technologies such as Microelectromechanical System (MEMS) because of the mixed-technology nature of microdevices. Typically, with a finite element method, the complexity of mesh generation grows significantly when more than one energy domain is involved. MEMS devices are typically mixed-domain systems which often involve at least two energy domains. Finite cloud method [2], a true mesh-

less method, is used in this paper to simulate electroosmotic transport.

There has been a growing interest in developing reduced-order models for MEMS and Bio-MEMS. The motivation behind developing reduced-order models is that by gaining information from the transient behavior of a particular flow problem, additional simulations can be performed by reformulating the problem in terms of global basis functions that capture the transient behavior, significantly reducing the number of degrees of freedom [3]. This technique drastically reduces the computational time, while at the same time minimizing the loss in solution accuracy. This new model can then be used to test the effects of changing various parameters in the system with much reduced time.

In this paper, we focus on simulating electroosmosis, the means for bulk transport for many μTAS, using the finite cloud method. In particular, we develop new meshless formulations for analysis of the nonlinear Poisson-Boltzmann equation, the Stokes equations and Navier-Stokes equations. Finally, reduced-order models are constructed based on Karhunen-Loeve decomposition [4].

2   Governing Equations

The equations governing the distribution of charge in the electric double layer near a solution-capillary interface and the resulting fluid motion due to an applied potential difference are well-known([5]). Under the assumption that the zeta potential effects extend only on a small distance into the channel, the applied potential gradient can be assumed to have no effect on the charge distribution near walls. Therefore, we can separate the two potentials in the formulation of the problem.

The ζ-potential at the solution-capillary interface results in a ψ-field. The corresponding charge density, assuming a symmetric and single-charged salt, is given

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by:

$$\rho_E = -2Fc_0 \sinh\left(\frac{F\psi}{RT}\right) \tag{1}$$

where F is Faraday's constant, R is the gas constant, T is the temperature, and c_0 represents the intrinsic ionic concentration in the absence of a potential. Combining Equation (1) and Poisson's equation relating charge and potential, we obtain the Poisson-Boltzman equation:

$$\nabla^2\psi = \frac{2Fc_0}{\epsilon} \sinh\left(\frac{F\psi}{RT}\right) \tag{2}$$

where ϵ is the permittivity of the solution. Introducing the Debye length λ_D given by

$$\lambda_D = \left(\frac{\epsilon RT}{2F^2 c_0}\right)^{\frac{1}{2}} \tag{3}$$

Equation (2) can be reformulated as

$$\nabla^2\psi = \frac{1}{\lambda_D{}^2} \frac{RT}{F} \sinh\left(\frac{F\psi}{RT}\right) \tag{4}$$

The potentials applied at the ends of channel result in a ϕ-field whose distribution can be determined by solving the Laplacian

$$\nabla^2\phi = 0 \tag{5}$$

When the flow of interest lies within the Stokes limit and the convective terms of the Navier-Stokes equations are negligible, fluidic transport is modeled using the Stokes equation and the continuity constraint, with the effect of the electric field on the ions in the double layer being represented by a per-unit volume force vector, $\boldsymbol{F}$.

$$\mu\nabla^2\boldsymbol{u} - \nabla p = -\boldsymbol{F} \tag{6}$$
$$\nabla \cdot \boldsymbol{u} = 0 \tag{7}$$

In Equations (6) and (7), μ represents the fluid viscosity coefficient, and p is the pressure. The forcing term is defined as

$$\boldsymbol{F} = \rho_E \boldsymbol{E} = 2Fc_0 \sinh\left(\frac{F\psi}{RT}\right)(\nabla\phi) \tag{8}$$

For problems where the non-linear convective terms become significant, the full Navier-Stokes equations must be solved. The transient Navier-Stokes equations with the electric force term $\boldsymbol{F}$ are given as

$$\frac{\partial \boldsymbol{u}}{\partial t} + (\boldsymbol{u} \cdot \nabla)\,\boldsymbol{u} = \nu\nabla^2\boldsymbol{u} - \frac{1}{\rho}\nabla p + \frac{1}{\rho}\boldsymbol{F} \tag{9}$$
$$\nabla \cdot \boldsymbol{u} = 0 \tag{10}$$

where ν and ρ are the solution's kinematic viscosity and density, respectively. $\boldsymbol{F}$ is still given by Equation (8), although the electric field intensity may vary with time to control flow rates and directions.

3 Development of Reduced-Order Model

Employing the finite cloud method, we have developed a stabilized Stokes solver, that solves equation (4)-(7), and a semi-implicit multi-step NS solver (SIMS), that solves equations (4), (5), (9) and (10). In developing a reduced-order model, global basis functions must first be generated from a series of snapshots. Snapshots of nodal velocities and pressures are obtained by solving the full Navier-Stokes equations using the SIMS solver and stored at regular intervals into a matrix of the form (e.g., for u)

$$[\boldsymbol{u}] = \begin{bmatrix} \vdots & & \vdots \\ \boldsymbol{u}_1 & \cdots & \boldsymbol{u}_N \\ \vdots & & \vdots \end{bmatrix} \tag{11}$$

where N is the number of snapshots. As shown by Hung et al [3], the global basis functions (or eigenmodes) that compose the reduced-order model can be taken as the columns of $\boldsymbol{U}$ from the singular value decomposition:

$$[\boldsymbol{u}] = \boldsymbol{U}\boldsymbol{\Sigma}\boldsymbol{V}^T \tag{12}$$

where $\boldsymbol{\Sigma}$ contains the corresponding eigenvalues. By inspecting the eigenvalues, the number of significant modes, for a particular state variable can be determined and those eigenmodes are the new global basis functions that will be used to reformulate the problem in terms of fewer parameters. For example, if the first four eigenvalues are dominant, then the first four columns of $\boldsymbol{U}$ are used as the new global basis functions. Thus the system's degree of freedom is greatly reduced. Given the new basis functions, the approximations to the functions can now be expressed as

$$u(x,y,t) = \sum_{i=1}^{q} \alpha_i(t)a_i(x,y) \tag{13}$$

$$v(x,y,t) = \sum_{i=1}^{r} \beta_i(t)b_i(x,y) \tag{14}$$

$$p(x,y,t) = \sum_{i=1}^{s} \gamma_i(t)c_i(x,y) \tag{15}$$

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where q, r, and s are the respective numbers of modes of u, v, and p determined to be significant. Each a_i, b_i, and c_i is one of the global basis functions, or modes, and each α_i, β_i, and γ_i is a time varying parameter. Together, these parameters and modes form the new numerical model.

Once these global functions are generated, the governing equations can be recast in terms of the reduced-order model. However, the resulting system of equations is overdetermined because the discretized equations are still satisfied at each node, but there are many fewer parameters. To obtain the desired solution, a Galerkin orthogonality condition is enforced [3]. That is, the residual error in the x and y components of the split momentum equation must be orthogonal to each basis function for u and v, respectively. Similarly, the error in the Poisson equation (second step of SIMS algorithm) is required to be orthogonal to each of the basis functions for p.

4   Numerical Results

4.1   Significance of Nonlinear Poisson-Boltzman Equation

The electroosmotic transport in a straight channel ($100\mu m$ wide and $5mm$ long) is first simulated. We apply a constant ζ-potential on the top and bottom walls, a potential at entrance reservoir 1, and hold exit reservoir 2 at ground. We have prescribed no-slip velocity conditions at the top and bottom walls, as well as $p = 0$ at the two reservoirs. The Debye length $\lambda_D = 5\mu m$ is used in order to be able to capture the behavior near the walls qualitatively without prohibitively dense node placement. Velocity distribution of this problem has an analytical solution given by Patankar and Hu [5] for the special case of small ζ-potential. The analytical solution is hereafter referred to as linear theory solution.

For the case of $\zeta = -1mV$, and $\phi_1 = 500V$ we are able to match the analytical result very well. For larger ζ-potentials, for which the linearity assumption $\sinh(\psi) \approx \psi$ no longer holds, our calculation matches the plug velocity (which is the velocity at the center of the channel) obtained from linear theory. However, the velocity variation closer to the wall differs from the linear theory prediction (see Figure 1). This result indicates that for a larger ζ-potential the use of linear Poisson-Boltzman equation is not justified. Defining the boundary layer thickness to be the distance from the wall to a position where the velocity is 90% of the plug velocity, Figure 2 shows the vari-
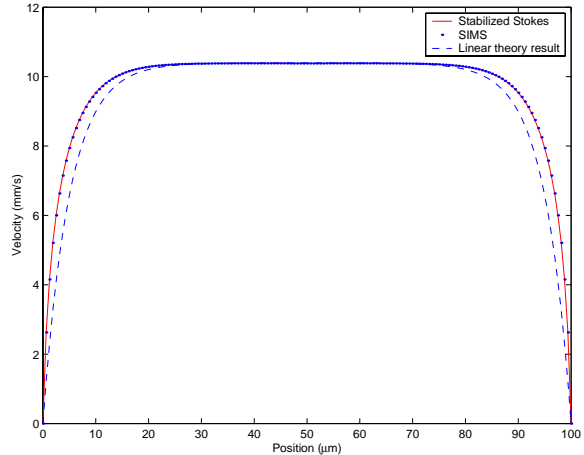

Figure 1: For $\zeta = -150mV$, linear theory predicts accurately the plug velocity but not the velocity variation near the wall

ation of the boundary layer thickness obtained with linear and nonlinear Poisson-Boltzman equations. For a given Debye length, the linear theory indicates that the boundary layer thickness is fixed while the nonlinear theory indicates that the boundary layer thickness decreases. A decreasing boundary layer thickness indicates a more rapid variation of velocity very close to the wall and thus a reduced hydrodynamic dispersion. In summary, a nonlinear Poisson-Boltzman equation should be used for large ζ-potentials to predict flow in the channel accurately.
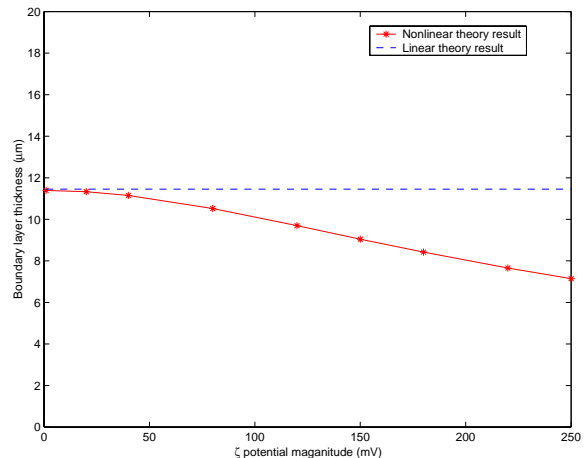

Figure 2: Non-linear variation of boundary layer thickness with ζ-potential magnitude. λ_D is fixed at 5 μm

4.2 Stokes vs Navier-Stokes

Cross-shaped intersection is a common component of electrophoretic separation systems. This geometry allows us to analyze global flow behavior in the channels as well as local behavior in the intersection. We have taken the origin to be the center of the intersection and set the dimensions as $W = 1.5mm$, $H = .9mm$, and $L = 30\mu m$. In the simulation, we set $\phi_1 = 1500V$, $\phi_2 = 0V$ and $\phi_3 = \phi_4 = 750V$. We compare the results of our two methods (Stabilized Stokes and SIMS) not only with previously published results [5], but also with each other in order to determine the validity of using the Stokes approximation to the Navier-Stokes equations. In particular, we analyze the significance of the convective terms in Equation (9), for a small and large ζ-potential.
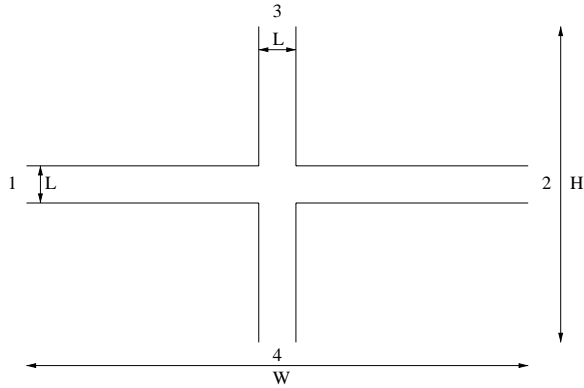

Figure 3: Cross channel geometry used for more complex analysis of electroosmotic flow characteristics

Since in the intersection, the flow is no longer axial, we expect the convective terms in the momentum equation to play a more important role than they will anywhere else in the domain (the convective term is zero far upstream and downstream of the bifurcation). Furthermore, there is no electroosmotic force driving the flow within the intersection. Flow within this region must therefore be due to viscous and inertial forces, as well as due to a small pressure gradient. By investigating the role of each term in the momentum equation at steady state, we have found that the convective terms are negligible for the case of small ζ, but significantly alter the character of the flow within the intersection for $\zeta = -150mV$. Within the main channel, the traditional Reynolds number, given by $Re = LU/\nu$, for the small ζ is 0.021 and for the large ζ is 3.204. Although these Reynolds numbers are slightly smaller within the intersection, the

effect of the convective terms at the higher Reynolds number is seen in the pressure contours shown in Figure 4. Calculations show that the pressure contours obtained from the Stokes equation and the NS equation are both symmetric and very close to each other for a small ζ, but for a large ζ, the pressure contours are no longer symmetric using the Navier-Stokes formulation because the convective terms have changed the flow characteristic within the intersection (see Figure 4). We conclude that in addition to being in the non-linear flow regime with respect to the ζ-potential, as shown in the previous section, we are also at the point where the Stokes equation is no longer valid to simulate fluidic transport within the intersection.
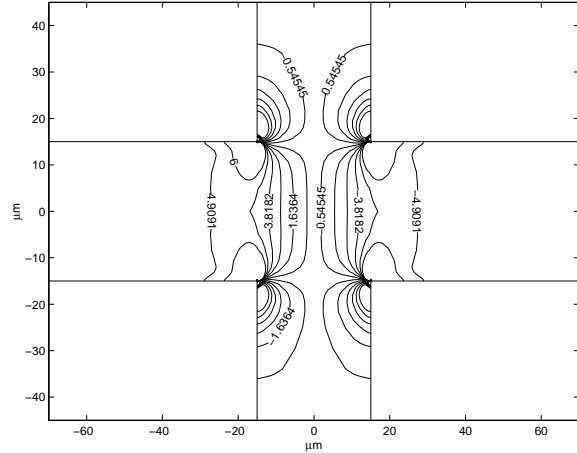
(a)
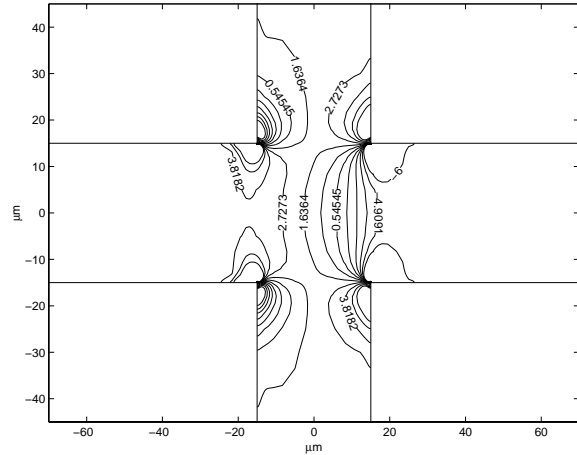
(b)

Figure 4: Pressure contours in Pa for $\zeta = -150mV$ using (a) Stabilized Stokes and (b) SIMS

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4.3 Reduced-Order Modeling of Electroosmosis in a Straight Channel

Because the pressure and v velocity are negligible for the straight channel geometry, the reduced-order model has been obtained by accumulating snapshots of the u velocity only. Furthermore, the equations governing v and p are not solved within the SIMS algorithm using the reduced-order basis. This procedure further reduces the number of parameters that must be obtained at each time step.

The first reduced-order model has been obtained by accumulating snapshots from the transient simulation of the straight channel (200 nm wide and 20 μm long) using $\zeta = -1.385$ mV and an electric field intensity of 10^3 V/m. Thirty snapshots have been obtained between the application of the electric field to stationary fluid and the steady flow profile, obtained approximately 30 ns later.

The contribution of each mode to the solution at 1 ns is shown in Figure 5. The first three modes are essential to capture the transient behavior of the flow. Calculations also show that only two modes are necessary to capture the steady flow behavior. In order for this model to be useful, it must be able to accurately predict the flow profiles for different values of ζ and electric field intensity than those used in obtaining the snapshots. Calculations show that the low-order model accurately predicts the behavior for a larger electric field intensity of 2×10^3 V/m. However, due to the nonlinearity of the Poisson-Boltzmann equation, the proper flow profile for $\zeta = -138.5$ mV cannot be generated using the basis functions obtained from snapshots taken with $\zeta = -1.385$ mV.

The same process of obtaining snapshots and generating the reduced-order model was conducted for a large ζ potential of -138.5 mV and a new reduced-order model was constructed. The first three modes capture the full time dependent flow characteristics for a large ζ potential. Again, the model can not predict the flow for a ζ potential much different from $\zeta = -138.5$ mV (e.g. $\zeta = -1.385$ mV). It is clear that the nonlinear Poisson-Boltzmann equation changes not only the potential profile, but also the shape of the velocity profile, when the linearity approximation $\sinh(\psi) \approx \psi$ is invalid.

In order to generate a much more useful reduced-order model, snapshots have been taken over a range of ζ values between -1.385 mV and -138.5 mV. Five snapshots over a 30 ns simulation time have been taken for each of the following values of ζ: -1.385 mV, -20 mV, -40 mV, -60 mV, -80 mV, and -138.5 mV. A total of 31 snapshots have been
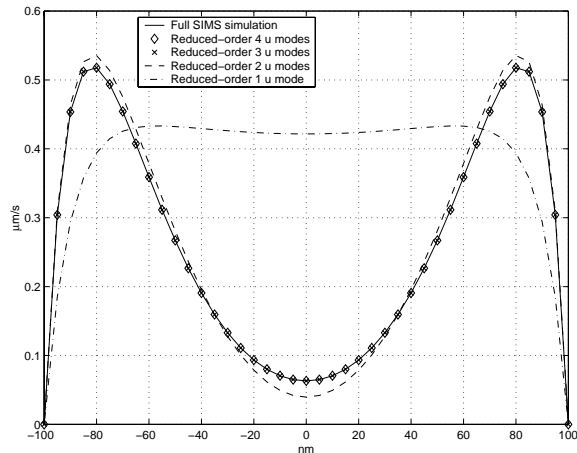

Figure 5: Comparison of reduced-order simulations to full SIMS simulation using different numbers of modes. Solutions are shown at 1 ns.

assembled in order to generate the new reduced-order model. The SVD of these snapshots has produced a fourth significant mode that allows for accurate simulation over the entire range of values of ζ, rather than being restricted to the linear regime. The first four modes for this more robust model are shown in Figure 6 along with their respective eigenvalues. The first three modes are similar to those obtained in the first model, but the fourth mode captures the nonlinearity of the profile for larger values of ζ. In Figure 7, this model using four modes is shown to match the full SIMS simulation steady-state results for a range of ζ potentials.

Thus a new reduced-order model has been constructed from snapshots of the velocity profile development for a range of ζ potentials. This new model can now accurately predict the flow characteristic within a straight channel for a wide range of ζ potentials and applied electric fields using much fewer degrees of freedom than the full SIMS simulation.

One more important feature of the reduced-order model is that it can speed up the simulation significantly while keeping reasonable accuracy. In the current simulation, 861 nodes were used. For 1200 steps of transient calculation, the full SIMS simulation costs 715s, and the reduced-order model costs around 13.6s (of which 2.1s were used to do the singular value decomposition). Thus the speedup factor is about 53. With increasing number of nodes or time steps, the speedup can be even more significant.

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Figure 6: The four dominant modes obtained from snapshots over a range of ζ in the straight channel. Corresponding eigenvalues are $3.49e - 3$, $6.22e - 5$, $2.5e - 5$, and $2.64e - 7$.

Figure 7: Results using new reduced-order model match full SIMS simulation results for a range of ζ including -1.385 mV, -40 mV, -100 mV, and -138.5 mV.

5   Conclusion

In this paper we have introduced a meshless method for electroosmosis simulation and have presented a reduced-order model based on Karhunen-Loeve decomposition. We have simulated electroosmotic transport in two geometries and identified the range of ζ-potential over which the linear approximation commonly used in literature is valid. We find that nonlinear Poisson-Boltzman equation is important for accurate prediction of the velocity profile when the ζ potential is large. We have also identified a combination of ζ potential and electric field intensity for which the Stokes approximation is insufficient to accurately predict flows within the intersection of the cross geometry. The reduced-order model developed shows excellent adaptability to a wide range of operating conditions while speeding up the simulation significantly.

Acknowledgment

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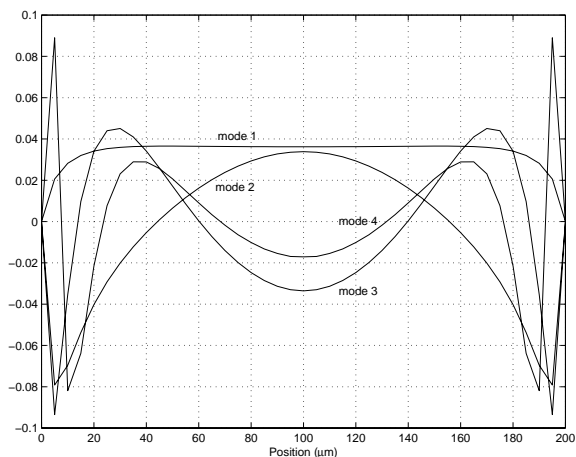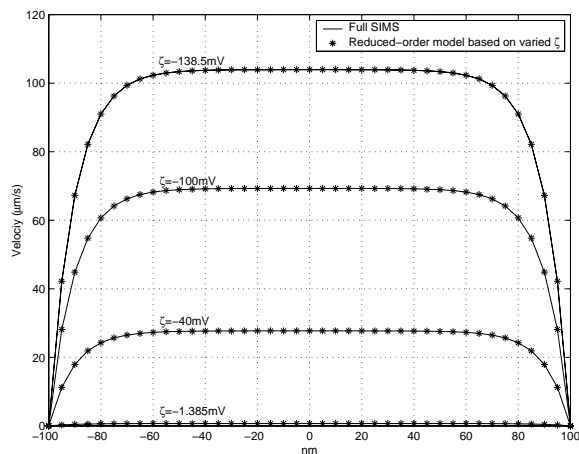[5] N. A. Patankar and H. H. Hu. Numerical simulation of electroosmotic flow. *Anal Chem*, 70:1870–1881, 1998.